

Topological phases in ZrTe_5 and chirality enabled quantum information systems

Qiang Li

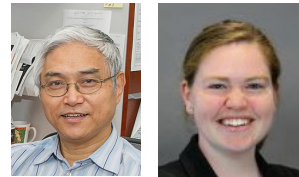
Department of Physics and Astronomy, Stony Brook University

Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory

Acknowledgements:

Collaborators/Group Members at Brookhaven National Lab and Stony Brook University

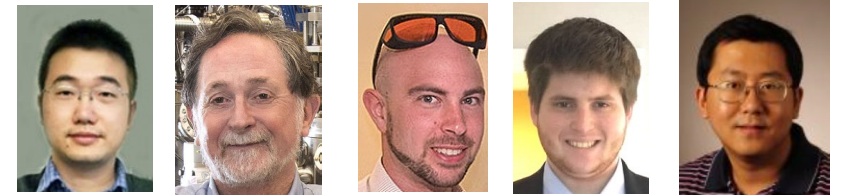
Single crystals
and thin films



Genda
Gu

Shannon
Lee

Optical and electron
spectroscopy (ARPES)



Mengkun
Liu

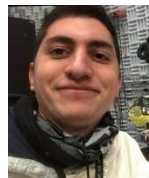
Peter
Johnson (R)

Dan
Nevola

Michael
Dapolito

Jigang Wang
(Ames Lab & Iowa
State University)

Quantum transport



Pedro
Lozano



Juntao
Yao

Theory/computation



Weiguo
Yi



Niraj
Arya



Alexei
Tsvelik



Dmitri
Kharzeev

This work was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-SC0012704.

Outline

- Chiral (Dirac/Weyl) semimetals and topological insulators
- Topological phase transitions
- Quantum computing with chiral fermions

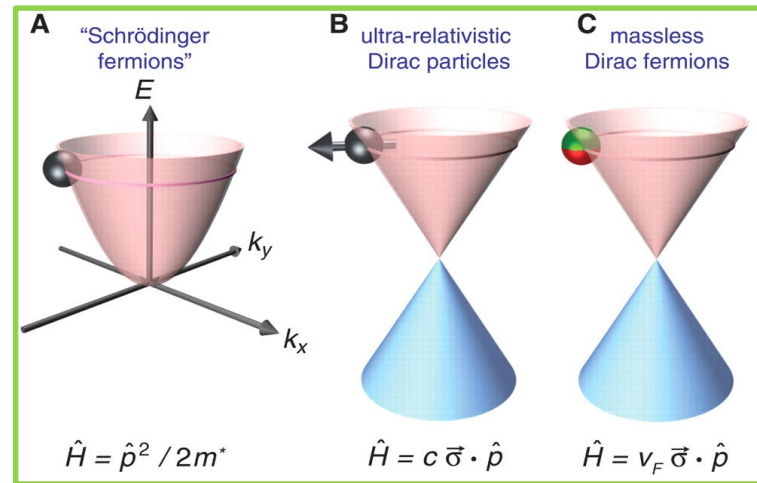
Chirality:

(electrons, quarks, and neutrinos)



Left-handed

Right-handed



A. K. Geim, Science 324,1530 (2009)

3D semimetals with linear dispersion

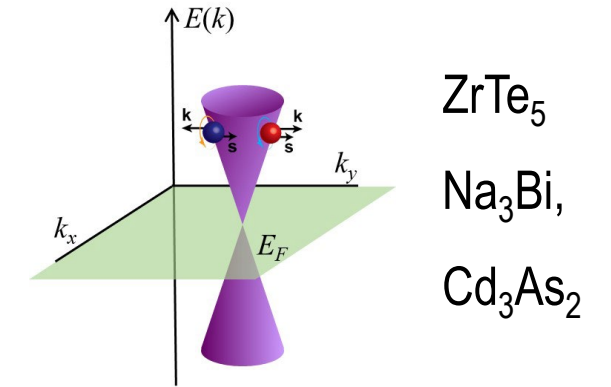
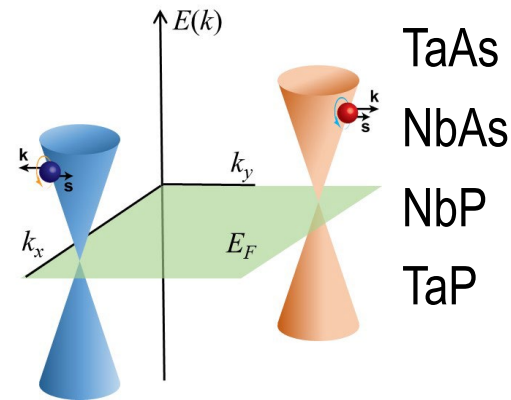
Weyl semimetal

(non-degenerated bands)

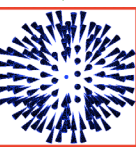
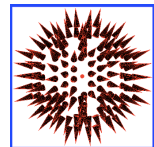


Dirac semimetal

(doubly degenerated bands)



- The Dirac point can split into two Weyl points either by breaking the crystal inversion symmetry or time-reversal symmetry.
- Each Weyl point acts like a singularity of the Berry curvature in the Brillion Zone – magnetic monopole in k -space

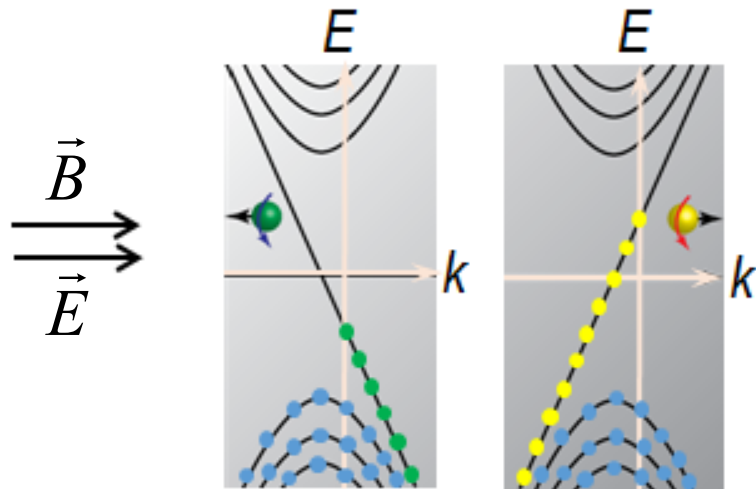




Dmitri Kharzeev
(SBU/BNL)

Chiral Magnetic Effect (CME) in Condensed Matters (CM)

The generation of electric current by the chirality imbalance between left- and right-handed fermions in an external magnetic field.



Chiral magnetic current: $\vec{J}_{CME} = \frac{e^2}{2\pi^2} \mu_5 \vec{B}$

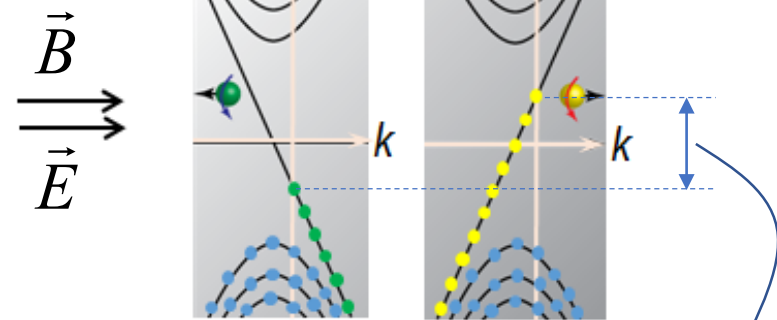
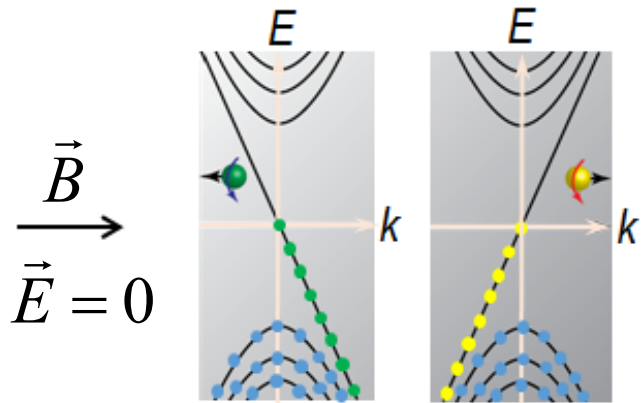
$$J_{CME}^i = \frac{e^2}{\pi\hbar} \frac{3}{8} \frac{e^2}{\hbar c} \frac{v^3}{\pi^3} \frac{\tau_v}{T^2 + \frac{\mu^2}{\pi^2}} B^i B^k E^k = \sigma_{CME}^{ik} E^k$$

$$\sigma_{CME}^{xx} = \frac{e^2}{\pi\hbar} \frac{3}{8} \frac{e^2}{\hbar c} \frac{v^3}{\pi^3} \frac{\tau_v}{T^2 + \frac{\mu^2}{\pi^2}} B^2 = \alpha(T) \cdot B^2$$

A negative longitudinal magnetoresistance (NLMR) at $(\vec{B} // \vec{E})$ in Dirac/Weyl semimetals

Chiral anomaly and chiral magnetic effect

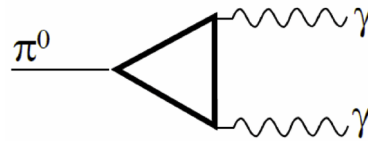
$$\vec{J}_{CME} = \frac{e^2}{2\pi^2} \mu_5 \vec{B}$$



$$\mu_5 \equiv \mu_R - \mu_L$$

Adler-Bell-Jackiw anomaly

Adler, Phys. Rev. 177, 2426 (1969)
Bell & Jackiw, Nuov Cim 60, 47–61 (1969)



Rapid decay of π^0 into two photons γ

Nielsen and Ninomiya (1983)

- Physics Letters B130, 389 (1983)

“The Adler-Bell-Jackiw anomaly and **Weyl** fermions in a crystal”

Son and Spivak (2013)

- Phys. Rev. B, 88, 104412 (2013).

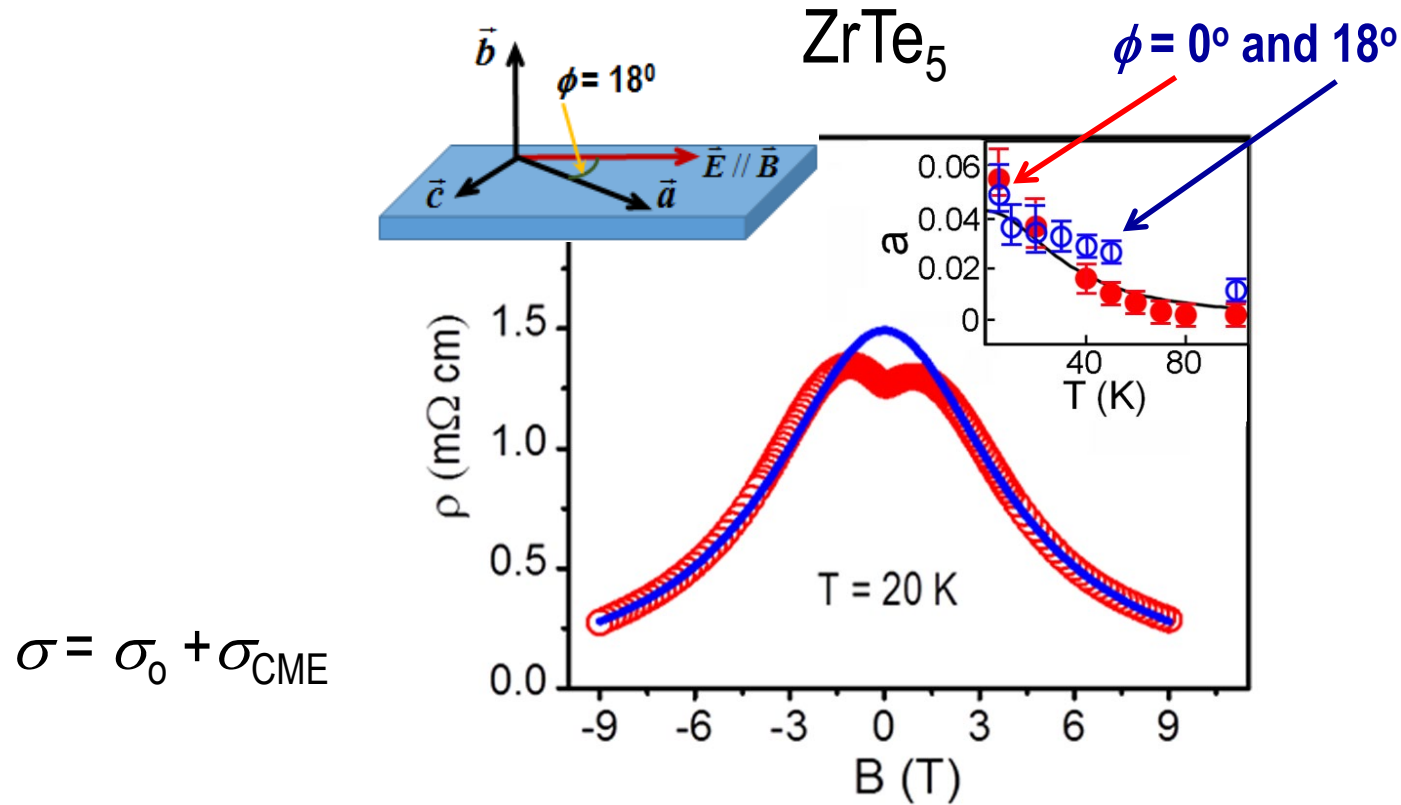
“Chiral anomaly and classical negative magnetoresistance of Weyl metals.”

Burkov (2014)

-Phys. Rev. Lett., 113, 247203 (2014).

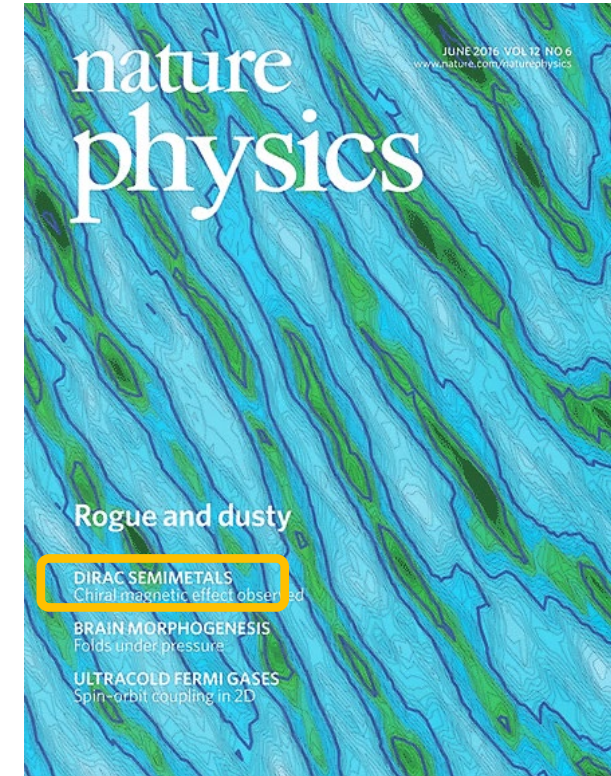
“Chiral anomaly and diffusive magneto-transport in Weyl metals”.

Discovery of chiral magnetic effect in ZrTe_5



$$\sigma = \sigma_0 + \sigma_{\text{CME}}$$

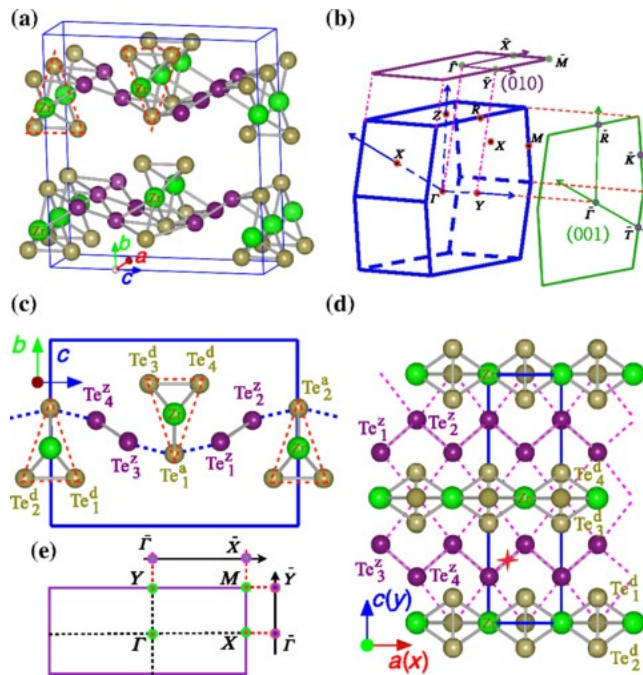
$$\sigma_{\text{CME}}^{zz} = \frac{e^2}{\pi \hbar} \frac{3}{8} \frac{e^2}{\hbar c} \frac{v^3}{\pi^3} \frac{\tau_V}{T^2 + \frac{\mu^2}{\pi^2}} B^2 = a(T) B^2$$



DIRAC SEMIMETALS
Chiral magnetic effect observed

Zirconium Pentatelluride ZrTe_5

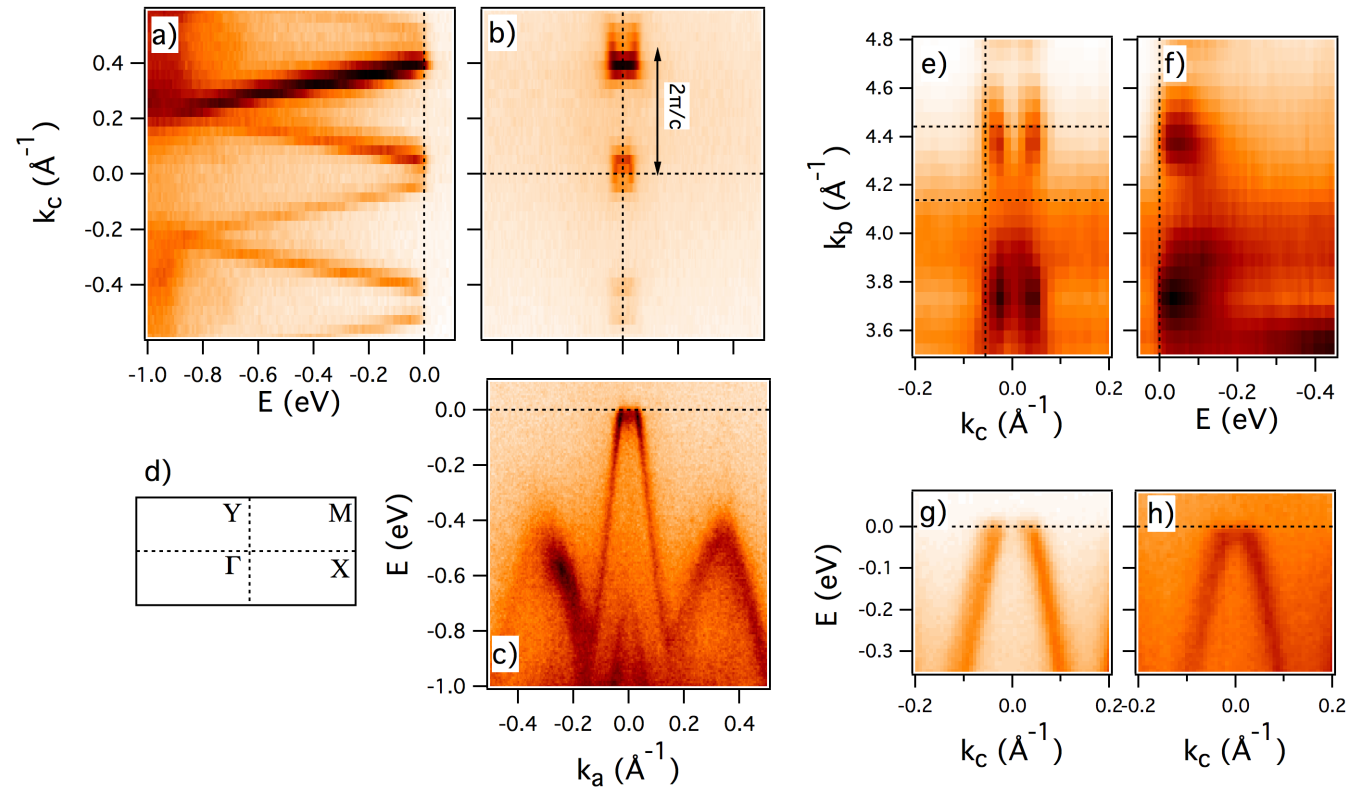
Crystal structure



2D topological insulator
(monolayer – prediction)

Weng et al. Phys. Rev. X 4, 011002 (2014)

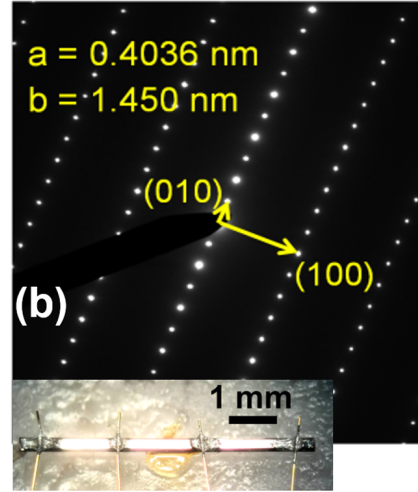
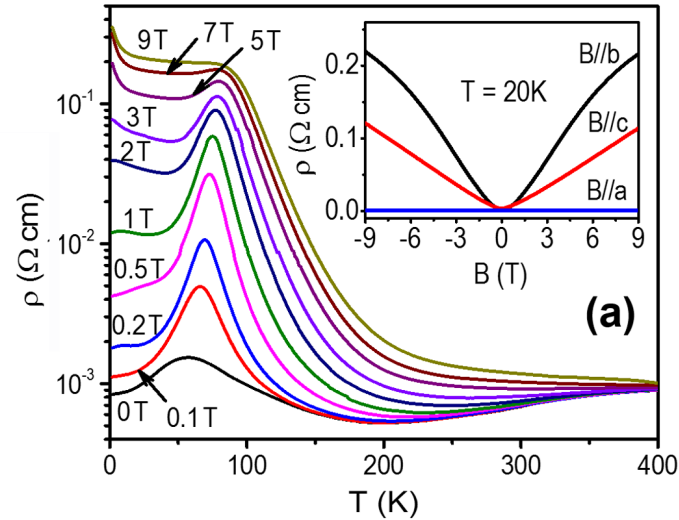
Electronic structure



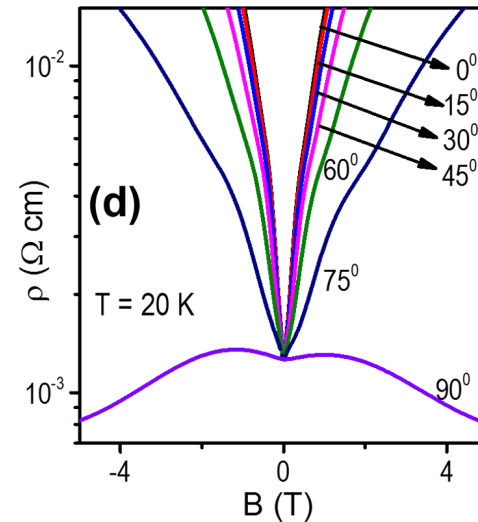
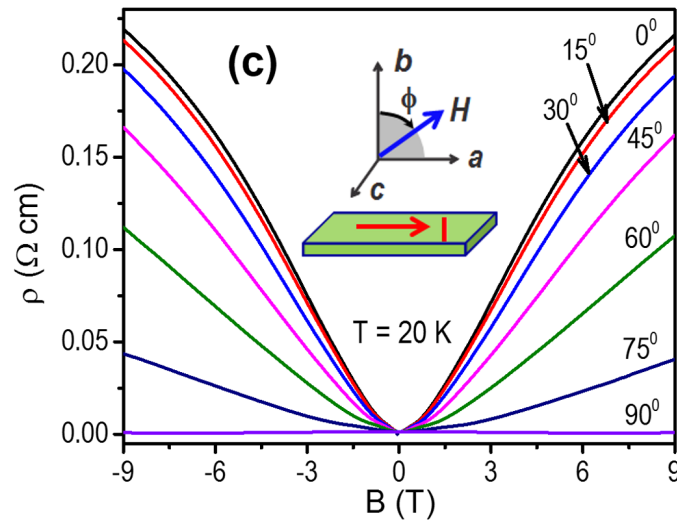
Dirac semimetal dispersion (ARPES)

Li et al. arXiv:1412.6543, Nature Physics 12 550 (2016)

Magneto-transport properties of ZrTe_5



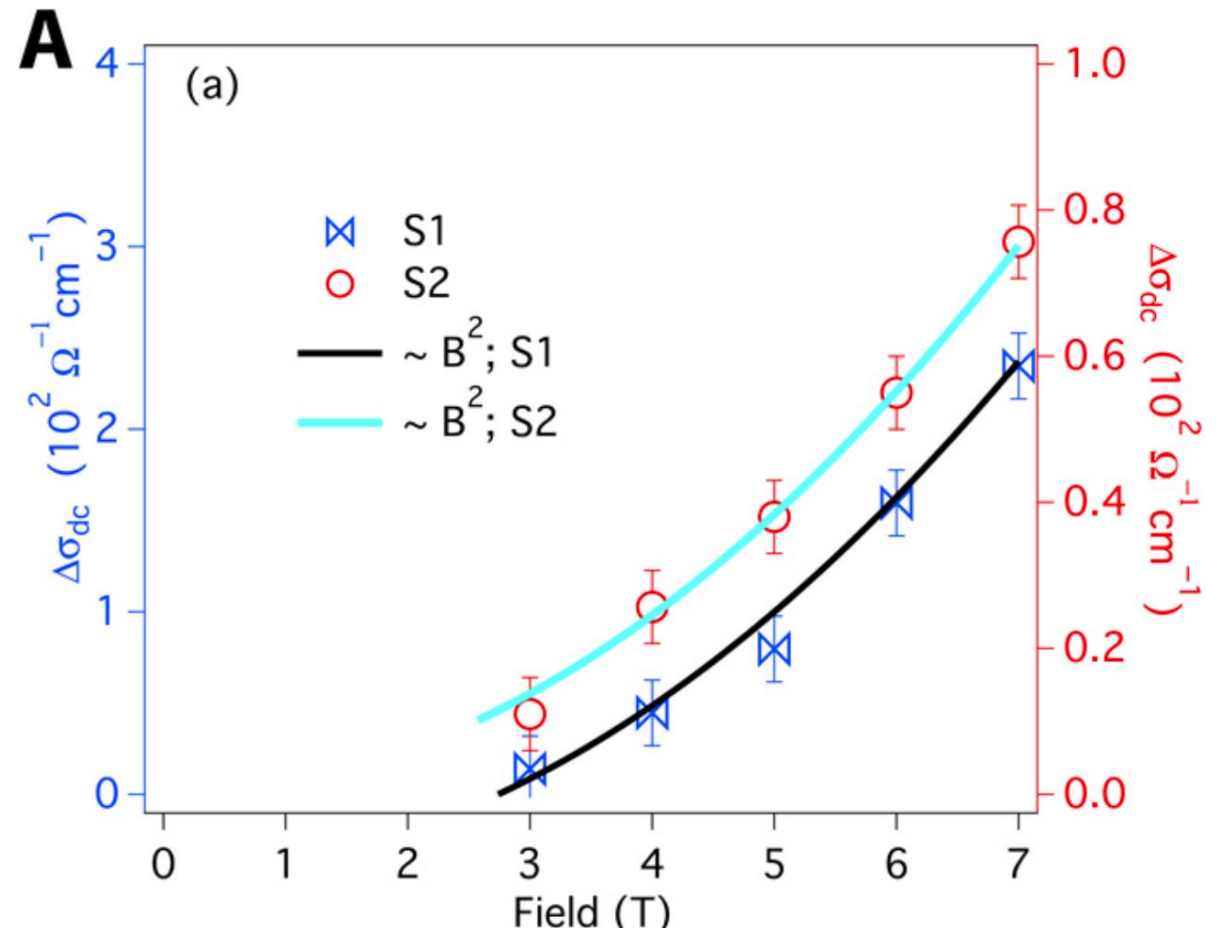
Measurable parameter from CME



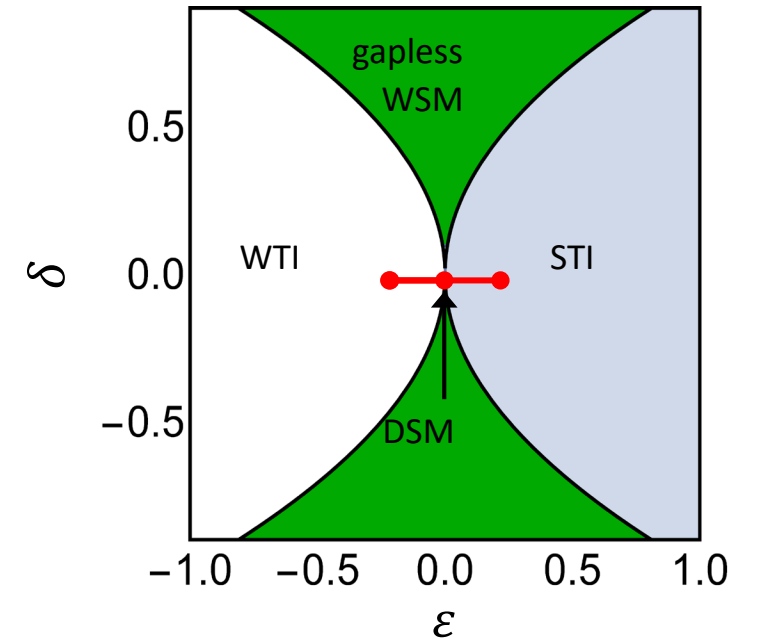
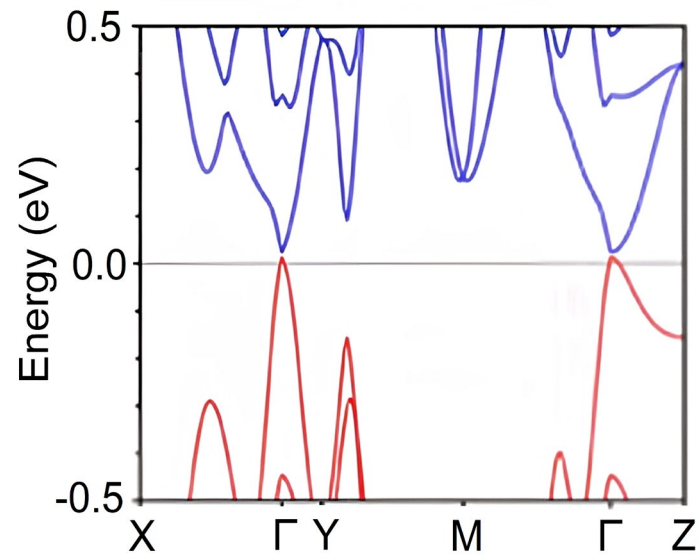
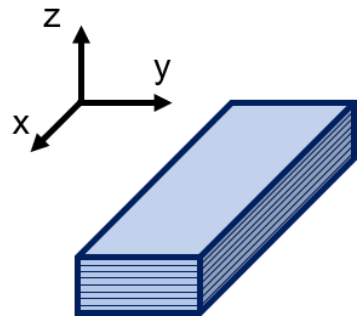
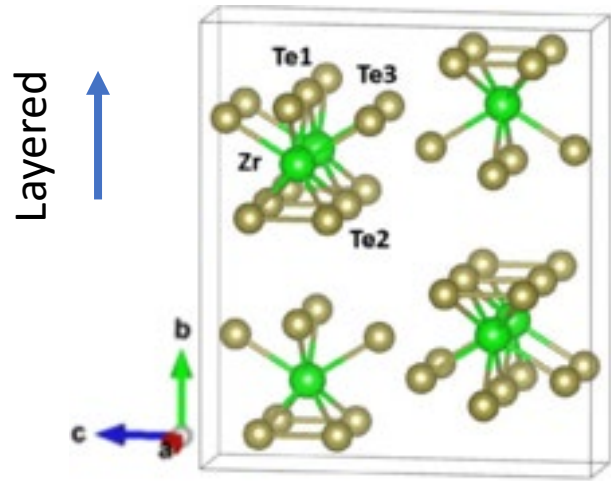
Large negative magnetoresistance
when $B//E$ ($\phi = 90^\circ$)

Magneto-terahertz spectroscopy (non contact) confirmed the chiral anomaly in a Dirac semimetal Cd_3As_2

“Intrinsic dc magnetoconductivity from chiral anomaly in sample S1 (blue) and sample S2 (red). In both samples, $\Delta\sigma$ follows B^2 ”

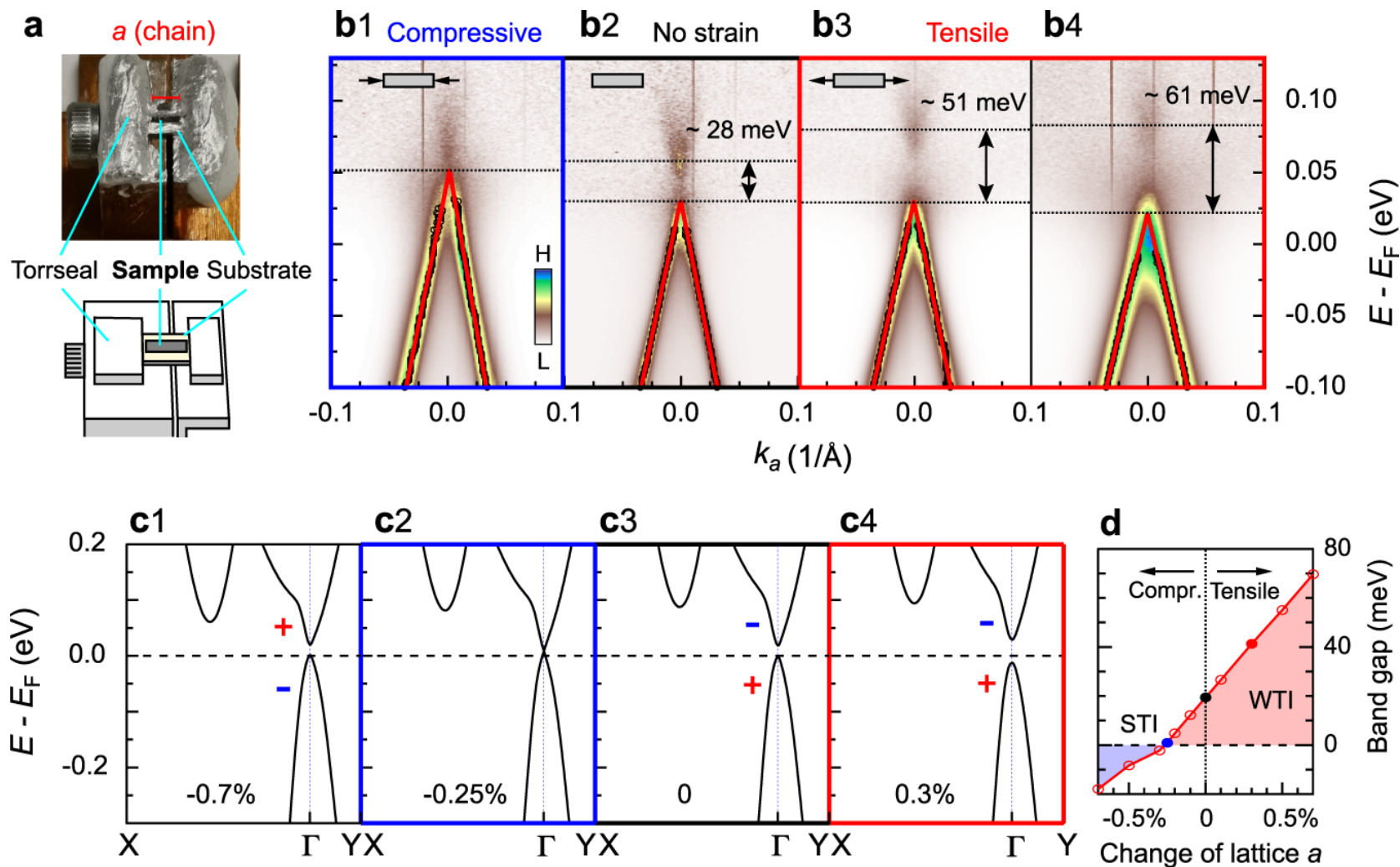


Topological states in ZrTe_5



Ref. P. Zhang, QL et al., Nat. Commun. 12, 406 (2021)
N. Aryal, QL et al., Phys. Rev. Lett. 126, 016401 (2021)

Strain Induced Topological Phase Transition in ZrTe_5



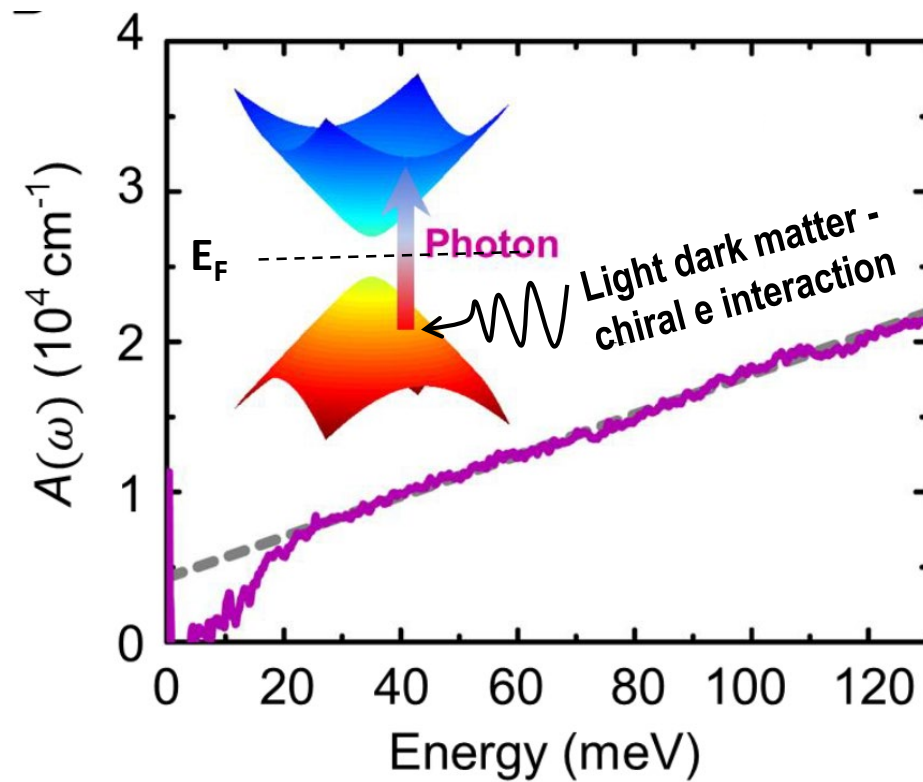
a) The strain device.

b) Bulk band gap change with compressive and tensile strain. The data are taken with p-polarized photons. The black markers are extracted from the MDC peaks, and the red solid lines are the fitting results

c) Calculated band structure with different lattice constant a . + and - signs indicate the parity of the two bands.

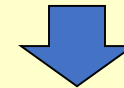
d) Calculated phase diagram with different lattice constant (strain). Blue, black, and red solid markers roughly indicate the experimental values in b.

ZrTe₅ - Light dark matter detection



- At no thermal excitation
- Fermi level in the gap Δ
(12.4 meV \sim 3 THz)

ZrTe₅

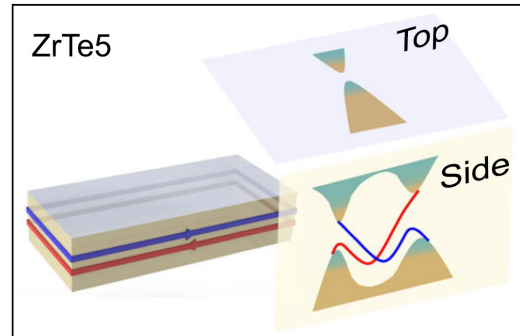


Light dark matter detection

More on topological states in ZrTe₅

3D weak topological insulator

Zhang, QL, et al. Nature Communications 12, 406 (2021)

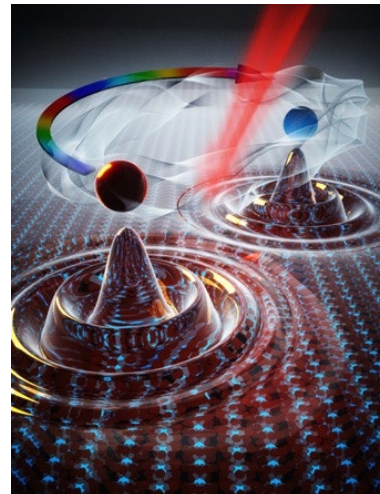


Dynamic Dirac/Weyl semimetal

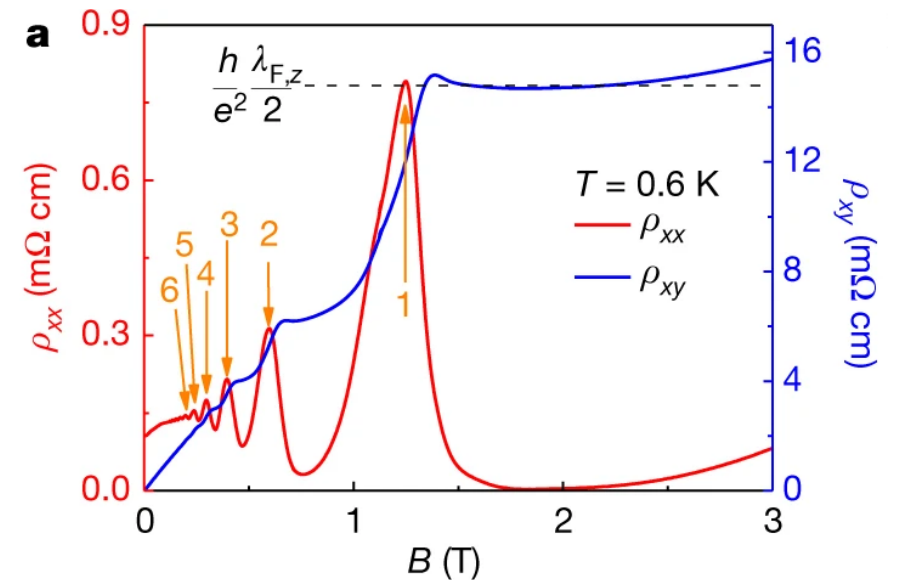
Aryal, QL, et al. Phys. Rev. Lett. 126, 016401 (2021)

Vaswani, QL, et al. Phys. Rev. X 10, 021013 (2020)

Luo, QL, et al. Nature Materials 20, 329 (2021)



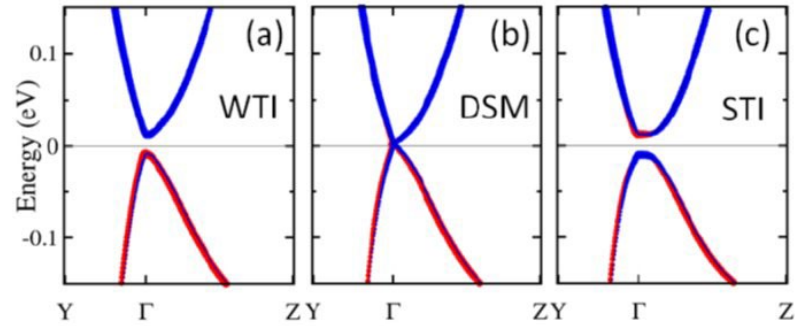
3D quantum Hall effect



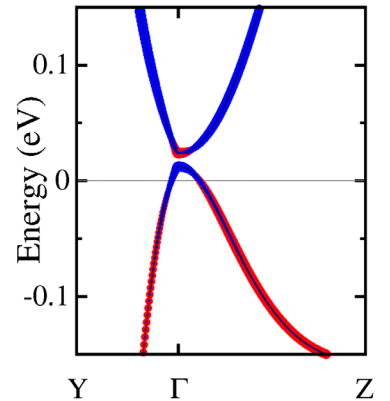
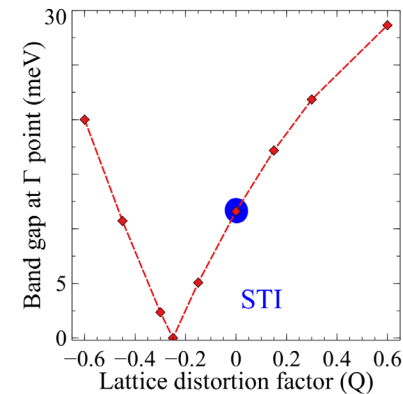
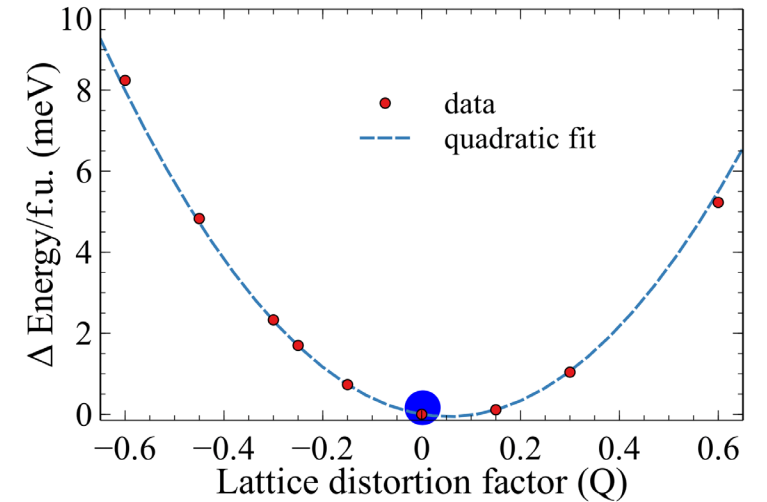
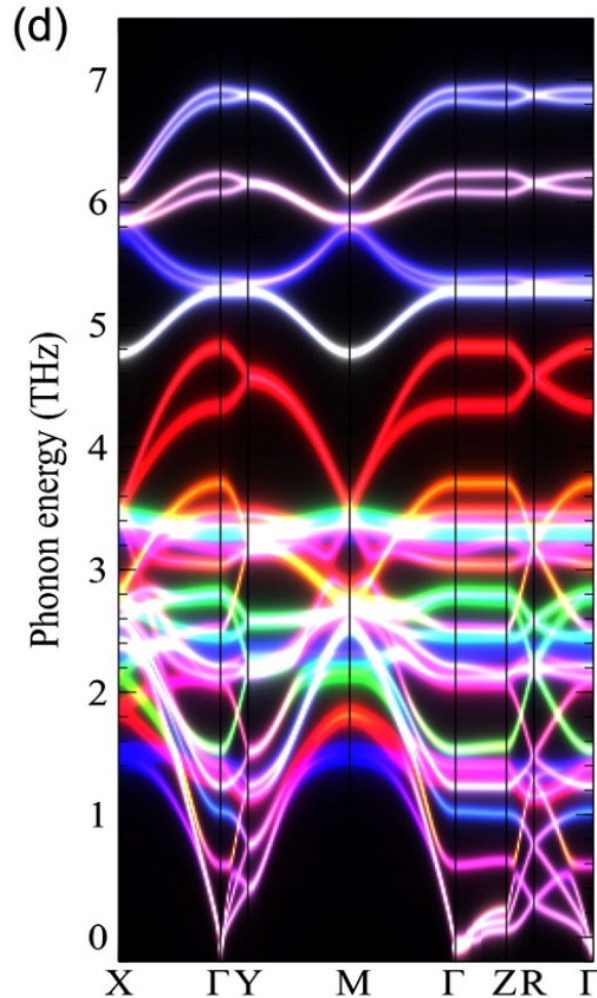
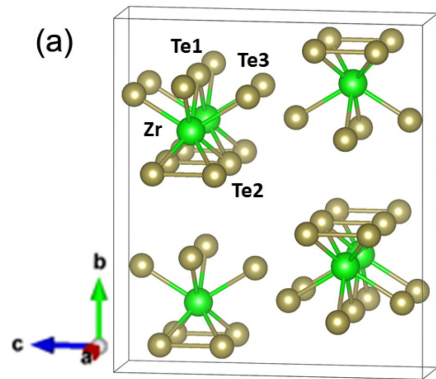
Tang et al. Nature 569, 537 (2019).

Galeski, QL et al. Nat. Commun.12, 1 (2021)

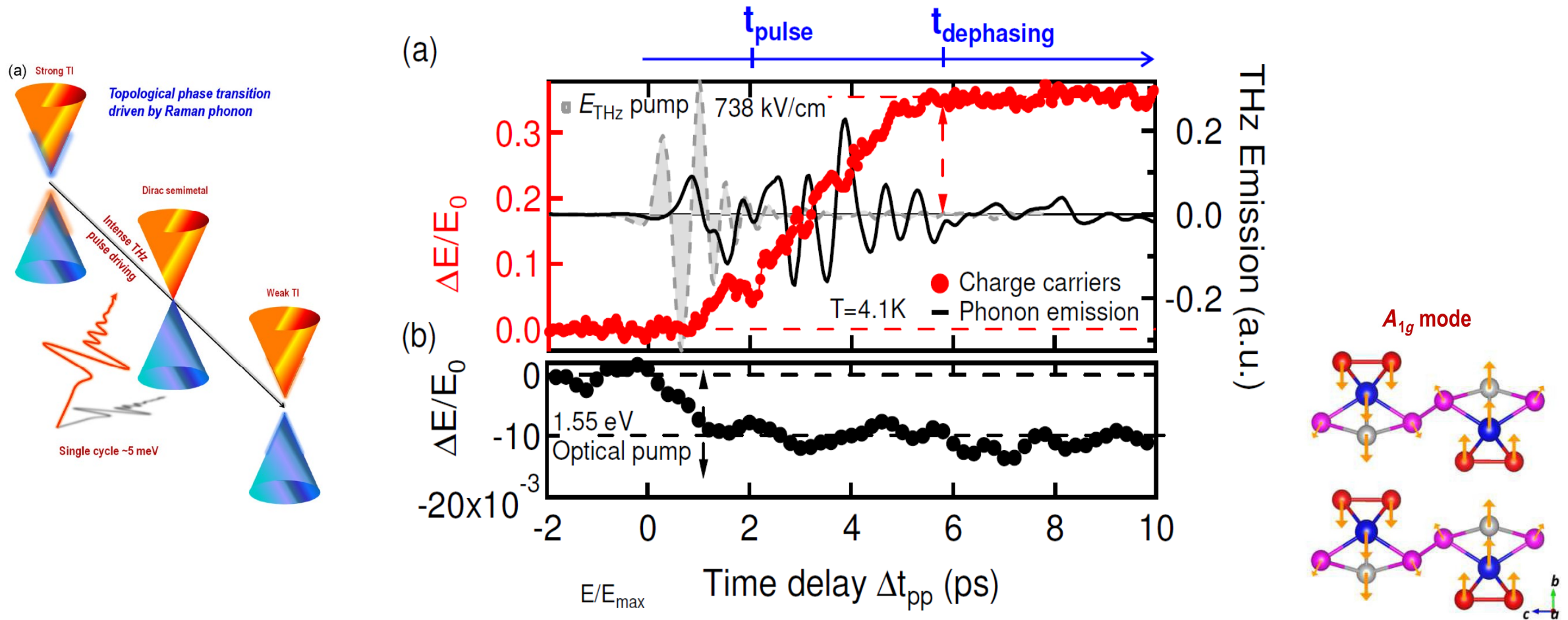
Coherent Phonon Control of Topological Phase Transition in ZrTe_5



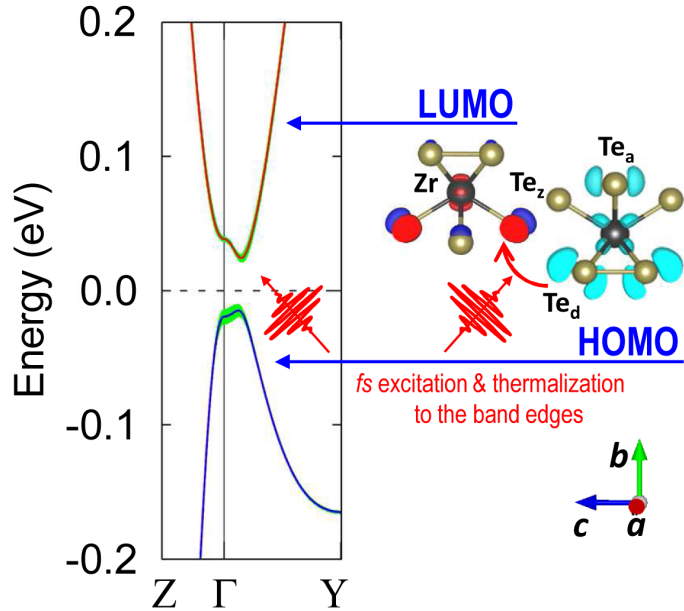
Evolution of the band structure around the Γ point for different values of the normal coordinate Q corresponding to the Ag-27 Raman-active phonon mode.



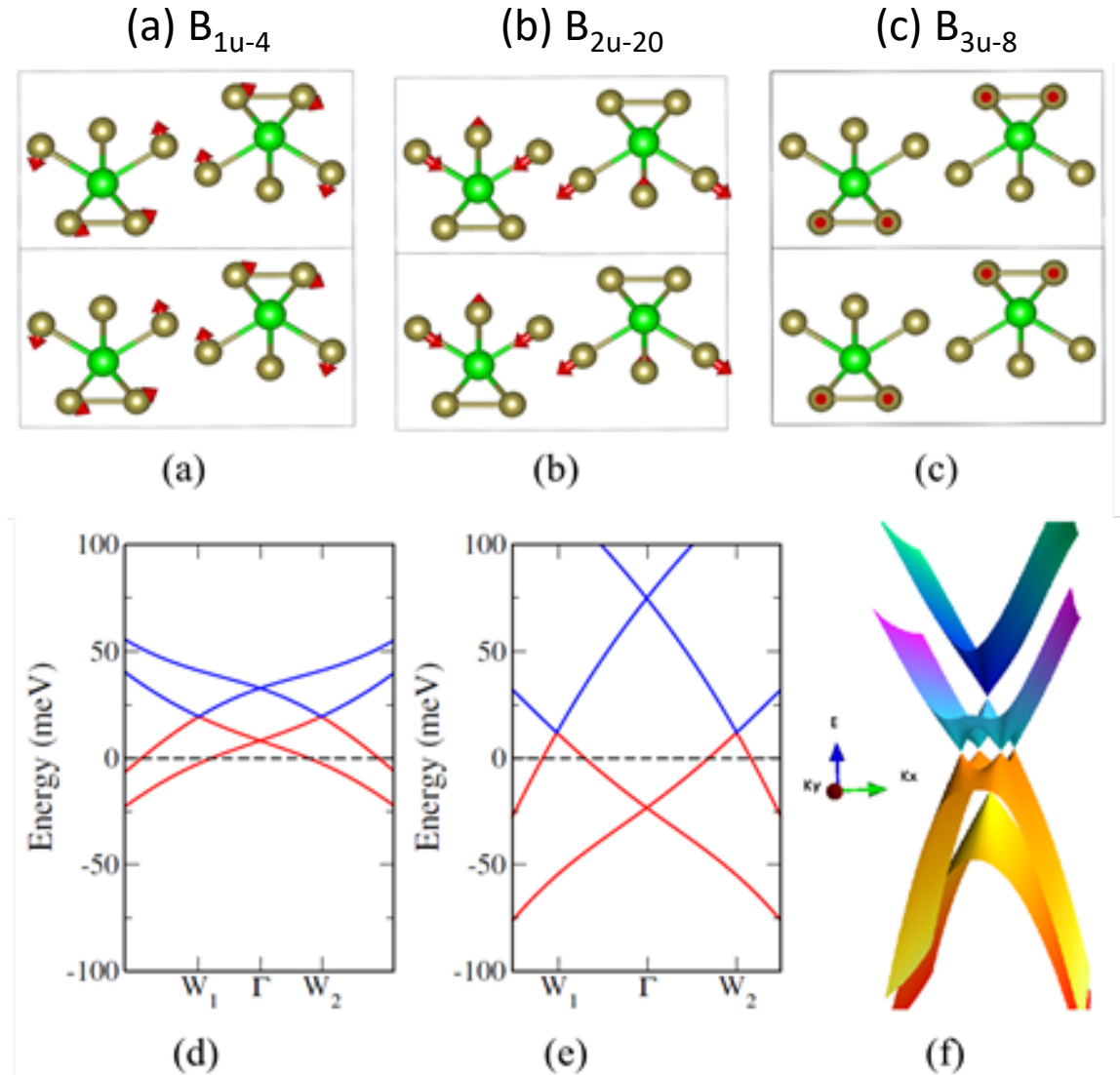
Light-Driven Ultrafast Topology Switching in ZrTe_5



Phonon induced Weyl phases in ZrTe_5^*

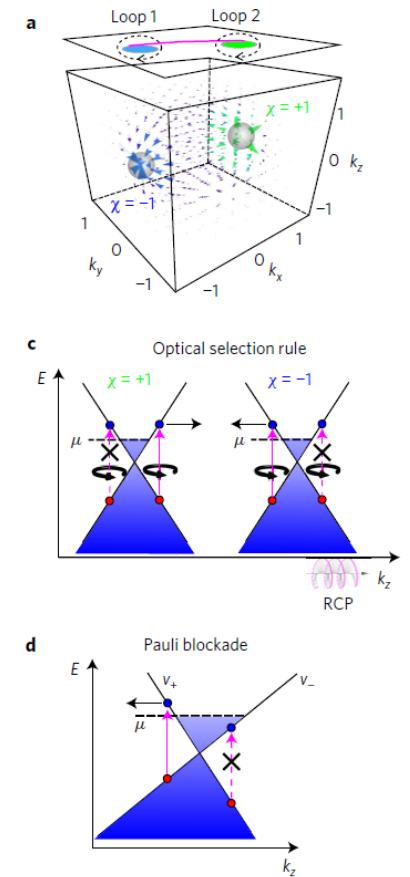
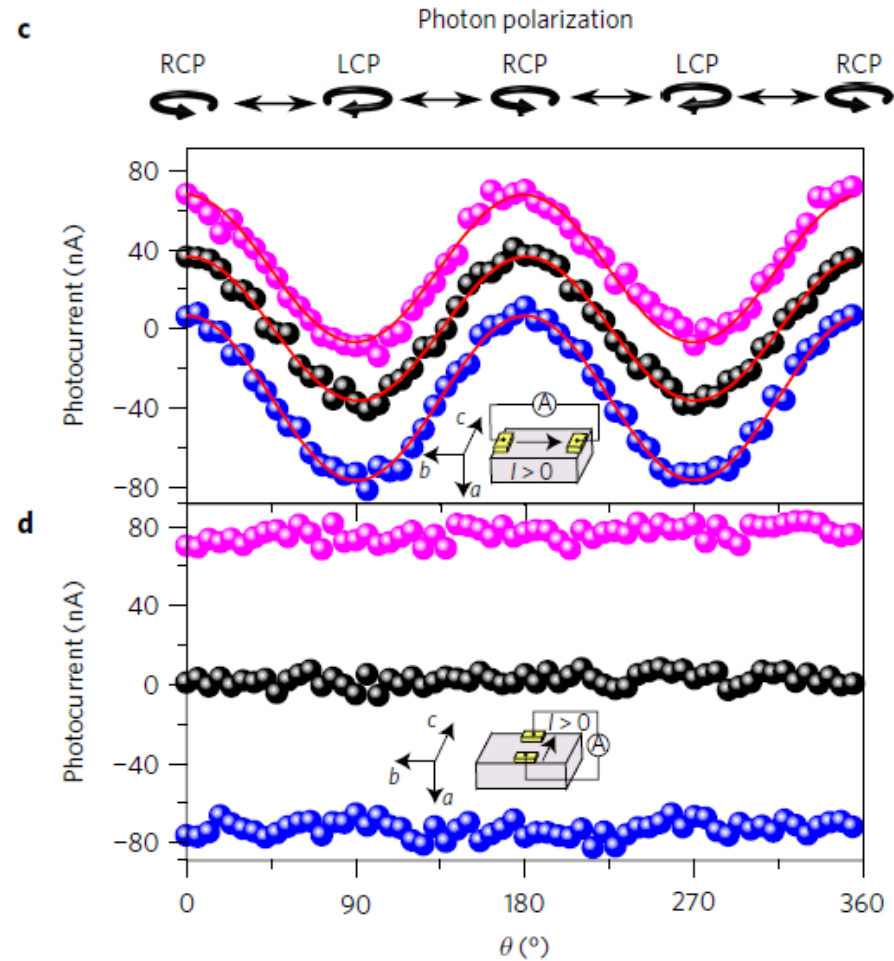
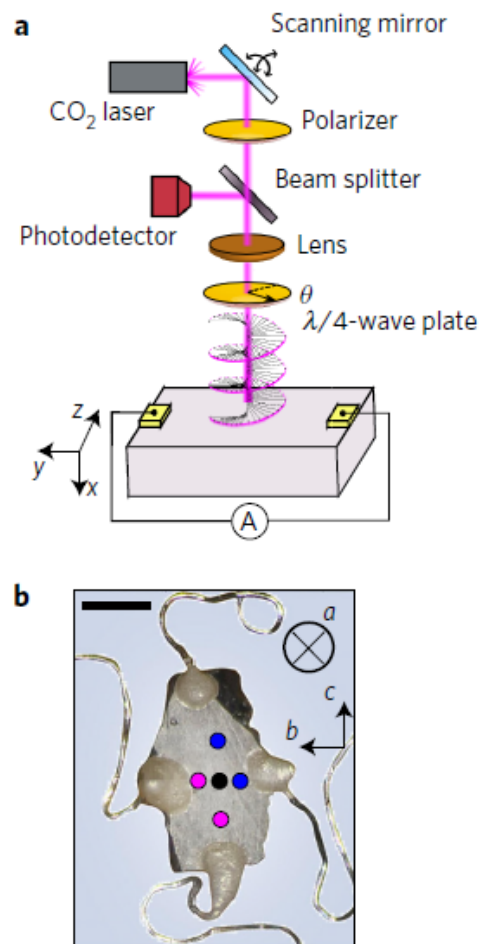


IR modes in ZrTe_5 projected on the b-c plane: (a) B_{1u-4} (b) B_{2u-20} and (c) B_{3u-8} ; (d), (e) Band structure along W_1 - Γ - W_2 direction for Q values of 1 and 4.5 respectively calculated from DFT for B_{1u-4} mode. (f), the bands forming the WPs are shown on the $k_x - k_y$.

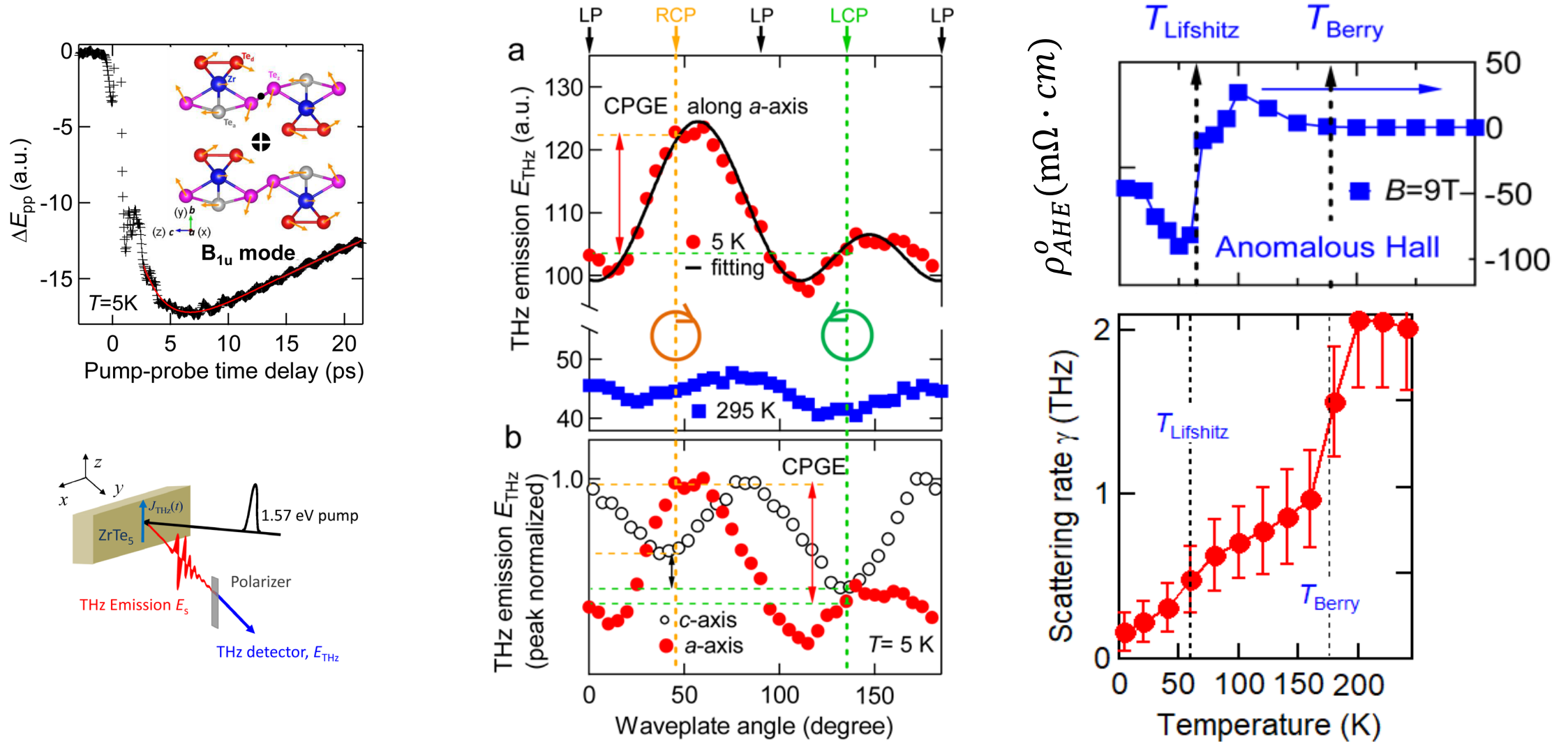


Detection and manipulation of chirality in Weyl semimetal TaAs

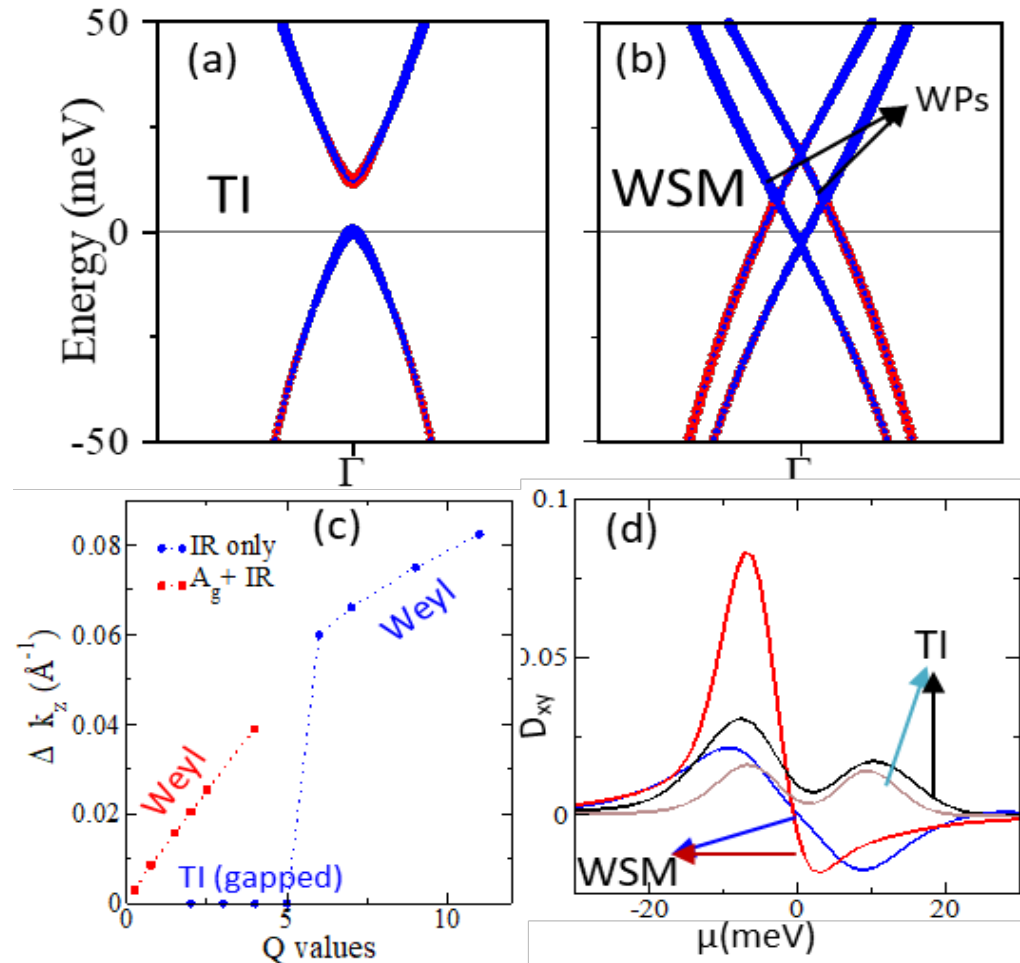
TaAs



A Light-induced Giant Dissipationless Topological Photocurrent in ZrTe₅



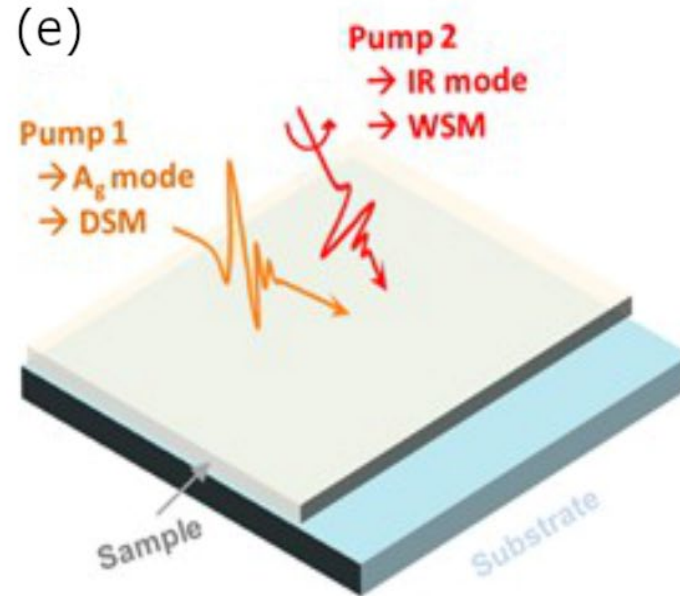
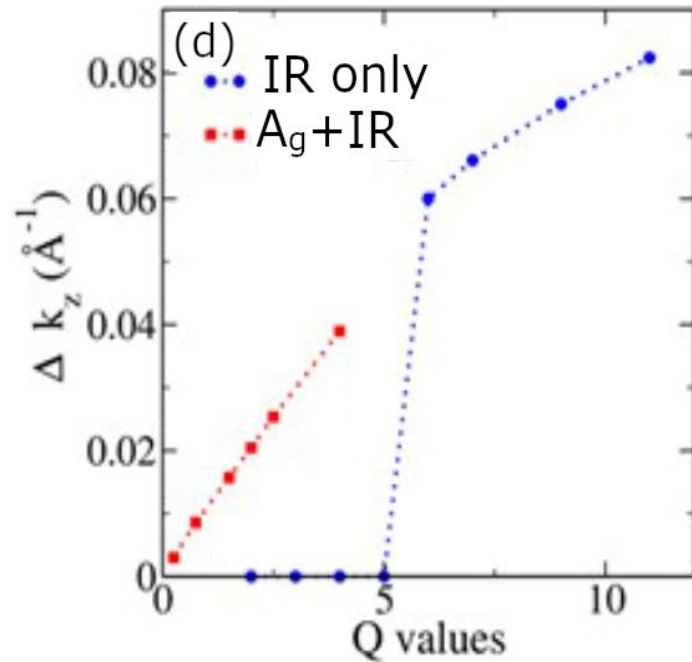
Tunability of Weyl phases by phonons



- The IR pumping threshold can be drastically reduced if used in conjunction with an A_g Raman-mode pumping that first drives the system towards the Dirac semimetal phase.

Figure (a, b) Evolution of the band structure of ZrTe₅ around Γ point with an IR mode lattice distortion $Q=0$ as a TI (a) and $Q=1.5$ showing Weyl points (WPs) (b). **(c)** Distance between the WPs when pumping from TI (blue) or DSM (red) phase. **(d)** Berry curvature dipole moment as a function of chemical potential for TI and WSM phases.

Reaching Weyl phases faster by Raman + IR phonons



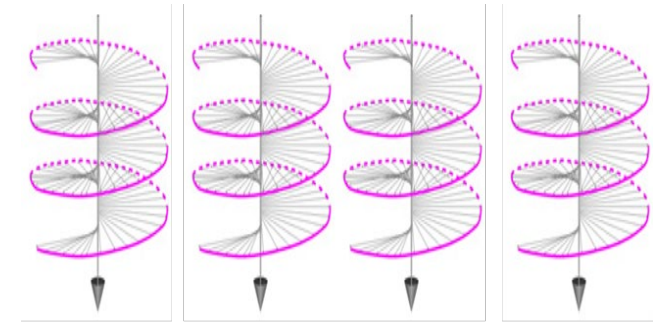
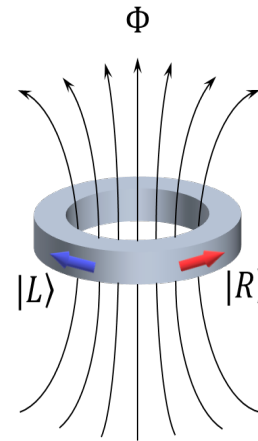
The IR pumping threshold can be drastically reduced if used in conjunction with an A_g Raman-mode pumping that first drives the system towards the Dirac semimetal phase.

Chiral Qubit*

Chiral Qubit is a micron-scale ring made of a Weyl or Dirac semimetal, with the two base states describing chiral fermions circulating along the ring clockwise and counter-clockwise. A fractional magnetic flux through the ring induces a quantum superposition. The entanglement of qubits can be implemented through the circularly polarized THz frequency electromagnetic fields.

$$\hat{H} = \hbar\omega \left(-i\partial_\theta + \frac{\Phi}{\Phi_0} \right) \hat{\sigma}_z$$

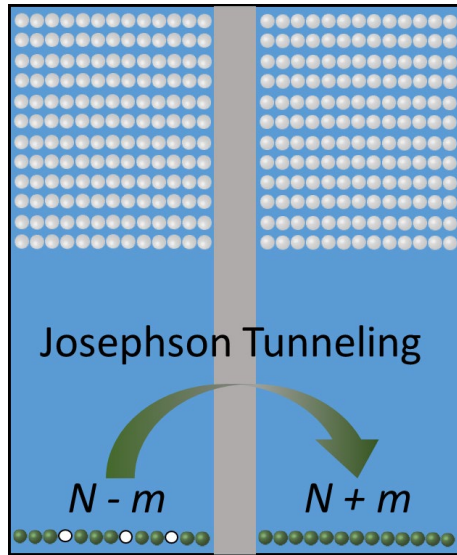
$$|0\rangle = \frac{1}{\sqrt{2}} (|R\rangle + |L\rangle), |1\rangle = \frac{1}{\sqrt{2}} (|R\rangle - |L\rangle)$$



$$\alpha |L\rangle + \beta |R\rangle$$

*D. Kharzeev and QL “Quantum computing using chiral qubits” United States patent #10,657,456 B1 (2020);
D. Kharzeev and QL “The Chiral Qubit: quantum computing with chiral anomaly” arXiv:1903.07133

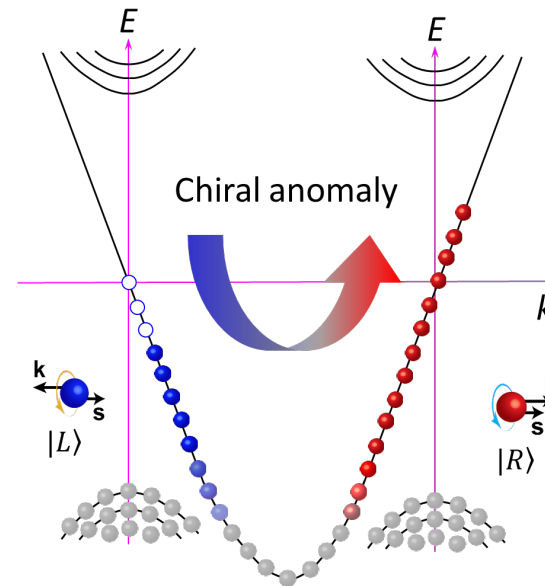
Superconducting qubit



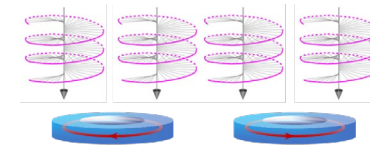
GHz energy gap
Microwave pulse

1 K ~ energy fluctuations 20 GHz

Chiral qubit

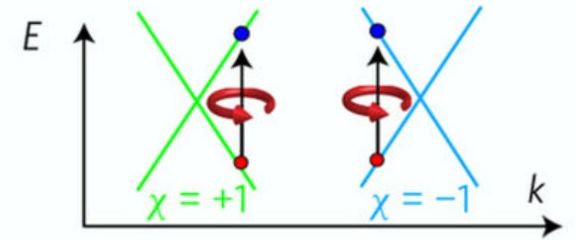


THz pulse

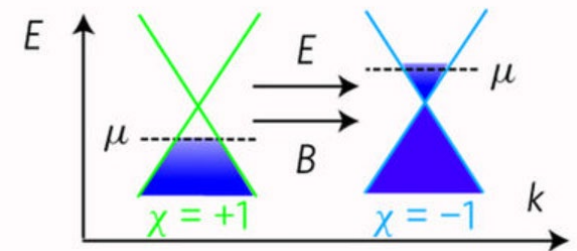


$\alpha |L\rangle + \beta |R\rangle$

Weyl—optical control



Weyl—electrical control



What do you need to build a quantum computer?

Di Vincenzo's Criteria*

1. A scalable physical system with well-characterized qubits.
2. Qubit initialization.
3. Long relevant decoherence times.
4. A “universal” set of quantum gates.
5. A qubit-specific measurement capability

Chiral qubit

None

~ OK, gate speed (THz) $> 10,000 \frac{1}{\tau}$

$$\tau > 100 \text{ ns}$$

Circular polarized light and duration

Circular polarization of THz emission

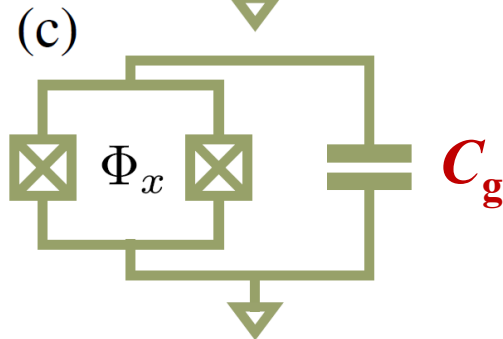
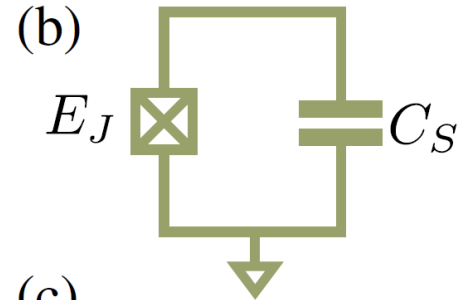
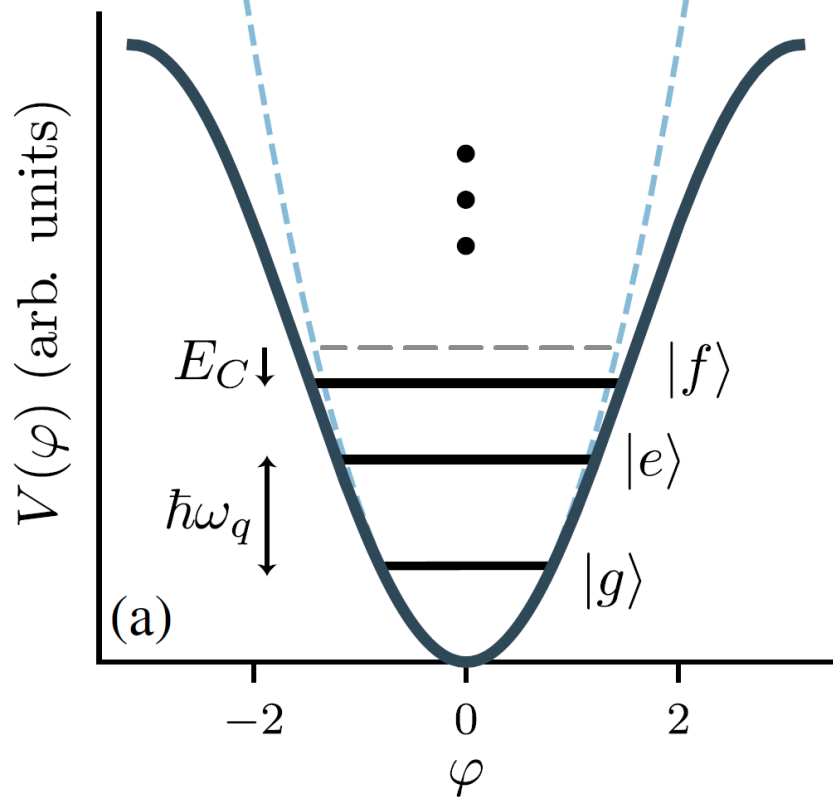
DiVincenzo Fortschritte der Physik 48, 771 (2000)



Stony Brook University

Superconducting quantum circuit

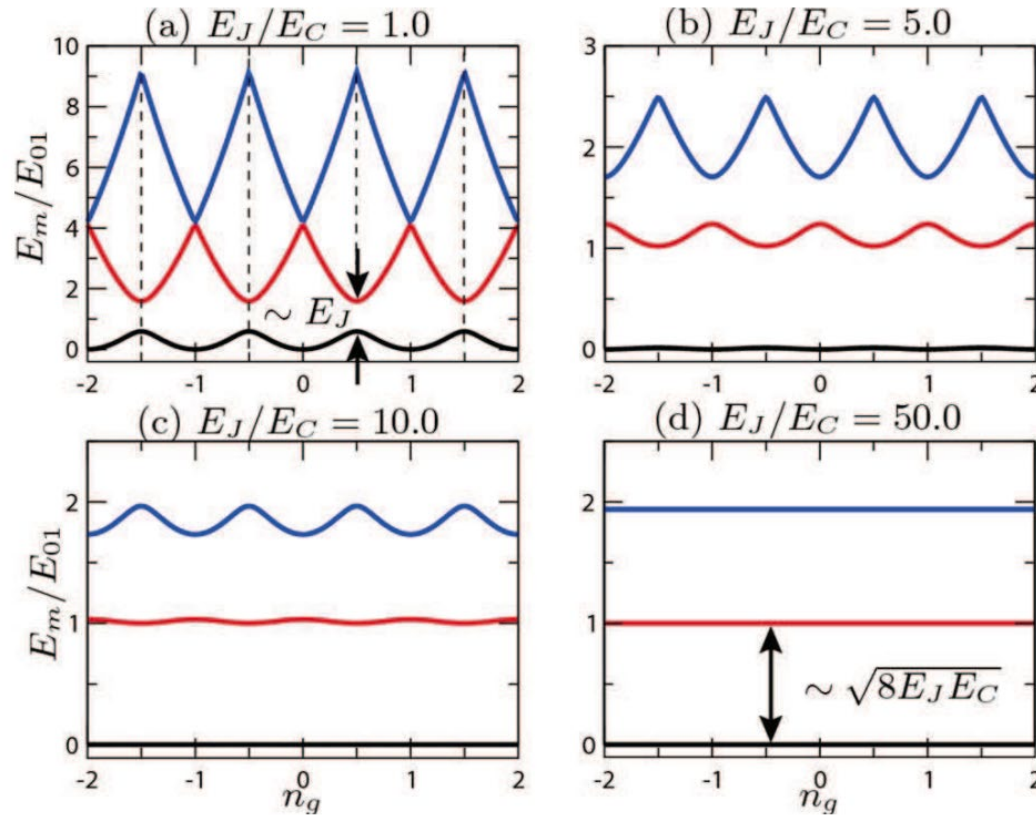
Nonlinear circuit – Artificial Atom



- If the nonlinearity and Q are large enough, we have an artificial atom
- If we restrict ourselves to $|g\rangle$ and $|e\rangle$, we have a qubit.
- By using a SQUID, the frequency of the transmon qubit becomes flux tunable.

The spectrum of \hat{H}_T is controlled by the ratio

$$E_J / E_C$$

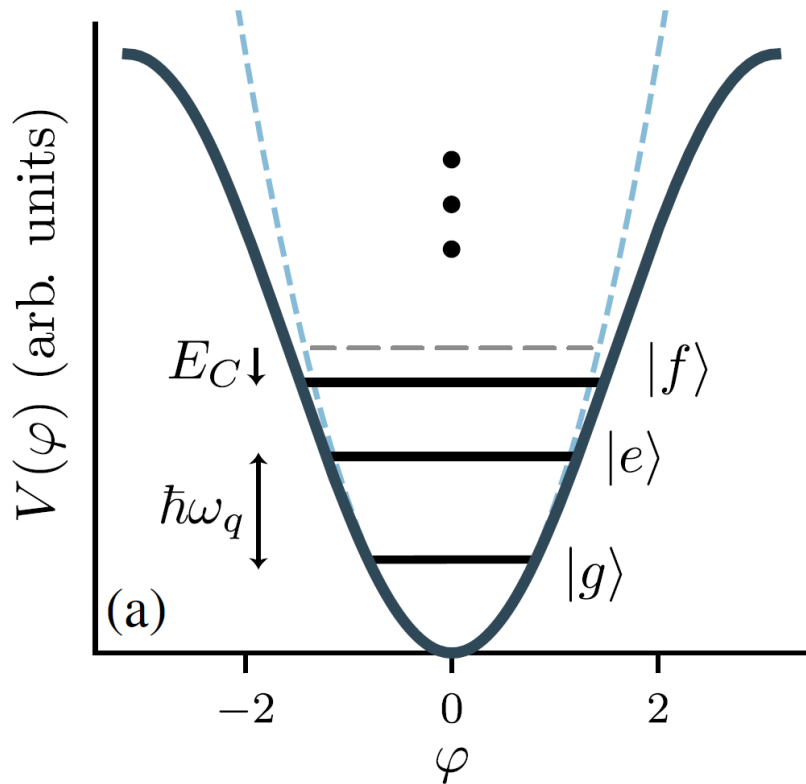


$$\begin{aligned} \hat{H}_T &= \frac{(\hat{Q} - Q_g)^2}{2C_\Sigma} - E_J \cos\left(2\pi \frac{\hat{\Phi}}{\Phi_0}\right) \\ &= 4E_C (\hat{n} - n_g)^2 - E_J \cos(2\pi \hat{\delta}) \end{aligned}$$

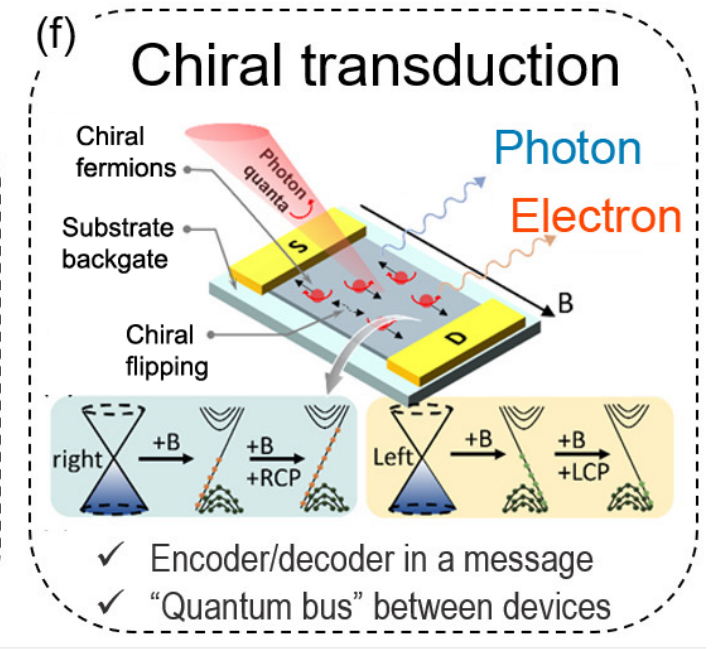
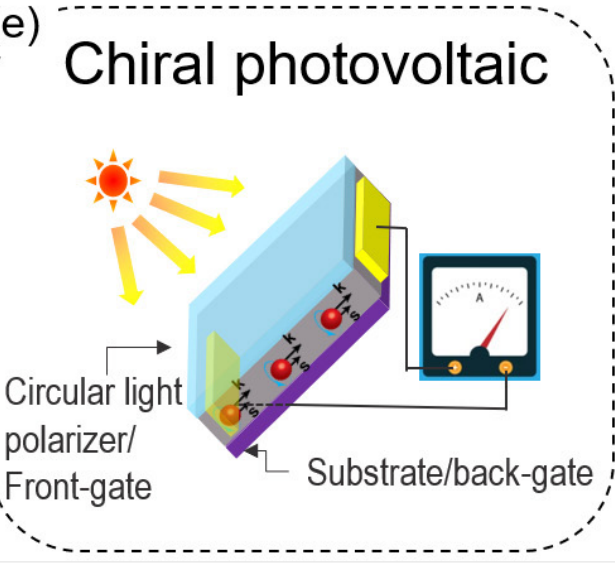
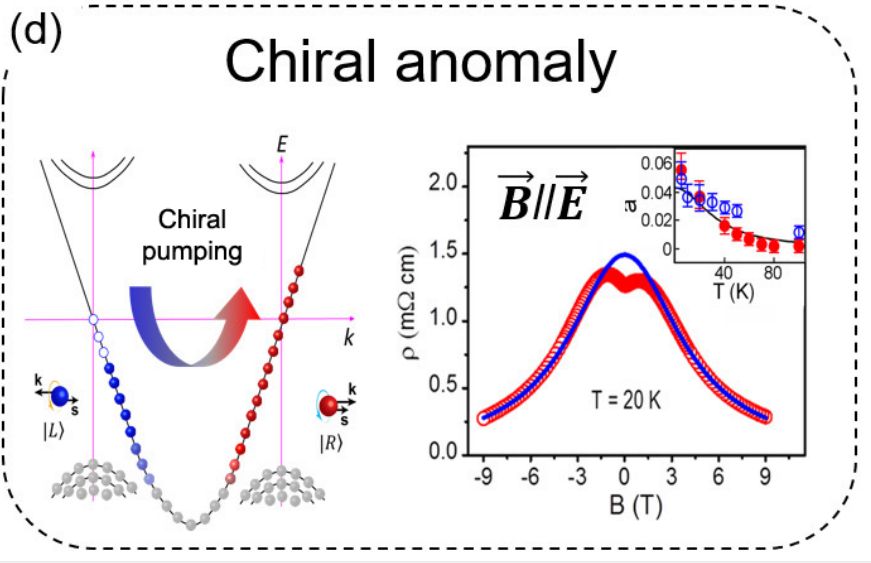
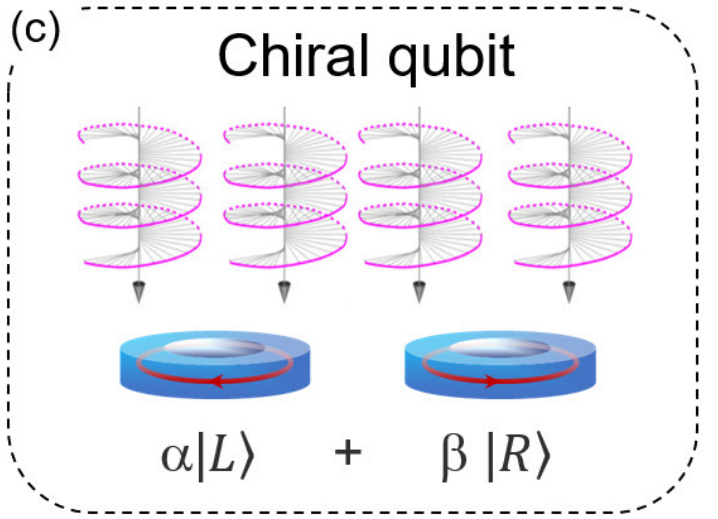
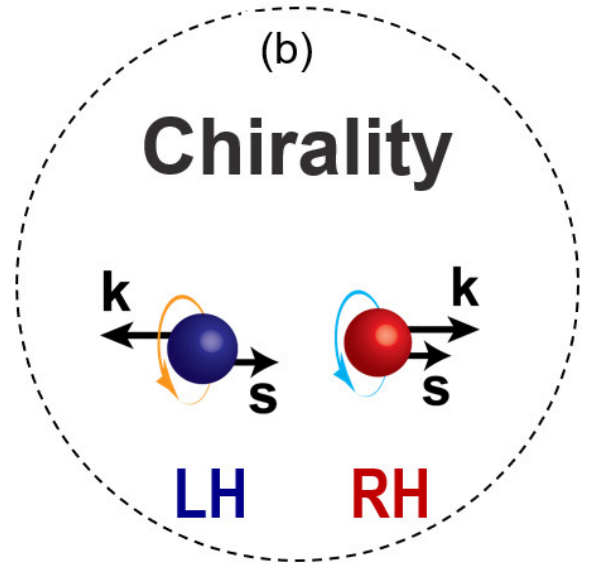
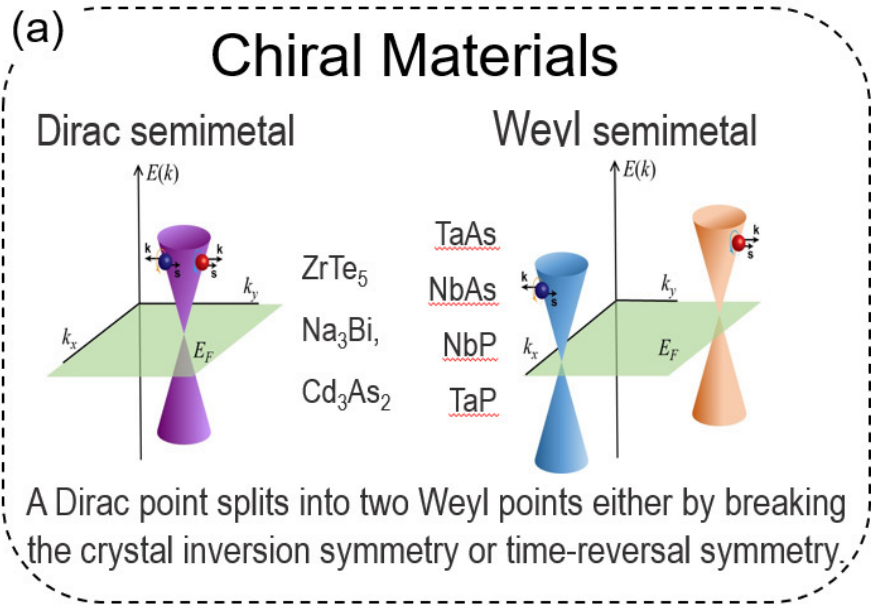
Frequency difference $\omega_j - \omega_0$ of the first three energy levels of the transmon Hamiltonian obtained from numerical diagonalization of the equation expressed in the charge basis $|n\rangle$ for different $\frac{E_J}{E_C}$ ratios and a fixed plasma frequency $\frac{\omega_p}{2\pi} = 5$ GHz. For large values of $\frac{E_J}{E_C}$ the energy levels become insensitive to the offset charge n_g .

$$\frac{E_J}{E_C} \ll 1 \sim \text{charge qubits}, \quad \frac{E_J}{E_C} \gg 1 \sim \text{transmon}, \quad (\text{Typically } \frac{E_J}{E_C} \sim 20-80)$$

Tunable chiral qubits



- Introduce nonlinearity, like a small mass term, m_g , ? => An artificial atom”
- Restricting ourselves to $|g\rangle$ and $|e\rangle$, we have a qubit.
- Gate m_g tuned controlled by strain, phonons, magnetic Weyl semimetal, magnetic impurity, etc



Concluding remarks

- Photoexcitation of phonon modes is shown to be an effective method to control topological states in ZrTe_5 . This should be applicable to other topological systems.
- Angular momentum coupling between circular polarized light and chiral fermions makes chirality effective quantum information carrier.